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A Prognosis of the Evaporation and Solvation Enthalpies of Organic Compouds on the Basis of the Topological Index 1χS

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Abstract

The influence of different types of intermolecular interactions, including dispersion, electrostatic, and specific, on the evaporation enthalpy of organic compounds was estimated. A series of quantitative relations between structural characteristics of a compound and the energy of its nonspecific solvation was established. It was shown that the evaporation enthalpy of more than 500 nonspecifically interacting compounds can be described with an accuracy to within ±2 kJ mol-1 by employing two descriptors, the topological index 1χS and the dipole moment. A new method for estimating the self-association enthalpy due to specific solvation was proposed.